Structural Materials

S. Maloy, C. S. Deo, M.R. James, S.G. Srivilliputhur, M.I. Baskes, D. Yeamans, T. Romero, M. Lopez
Los Alamos National Laboratory

M. Toloczko, F. Garner
Pacific Northwest National Laboratory

M. Okuniewski, J. Stubbins
U. Of Ill. (Urbana/Champaign)

G. Was
U. of Michigan

P. Rittenhouse, W. Sommer
TMC

AFCI Semi-annual Meeting
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Highlights ('03)

- Mechanical Testing and Microstructure
  - 3 pt. bend testing of proton irradiated 9Cr-1Mo and 316L at RT, 250, 350 and 500C.
  - Tensile and shear punch fixture were designed and constructed for testing in a hot cell.
- Data
  - Rev. 4 of Materials Handbook in final stages.
    - » Reviewed and finalized chapter on Tantalum
    - » Reviewed and Final Revisions are in progress on HT-9/EP-823 chapter.
  - International Collaborations
    - » Attended TRADE target workshop in Karlsruhe, Germany in May 2003
    - » Attended Megapie PIE workshop in Villigen, Switzerland in May 2003
- Atomistic Modeling of He in Body-centered Cubic (BCC)-Fe
  - Established parameters for a bcc (body-centered cubic, this is the basic structure of F/M steels) Fe-He system at different temperatures and He pressures.
  - Initiated trial low energy Primary Knock-on Atoms (PKA's) (5keV) in Fe and Fe-He systems.
  - Calculated migration energies of He in BCC Fe.

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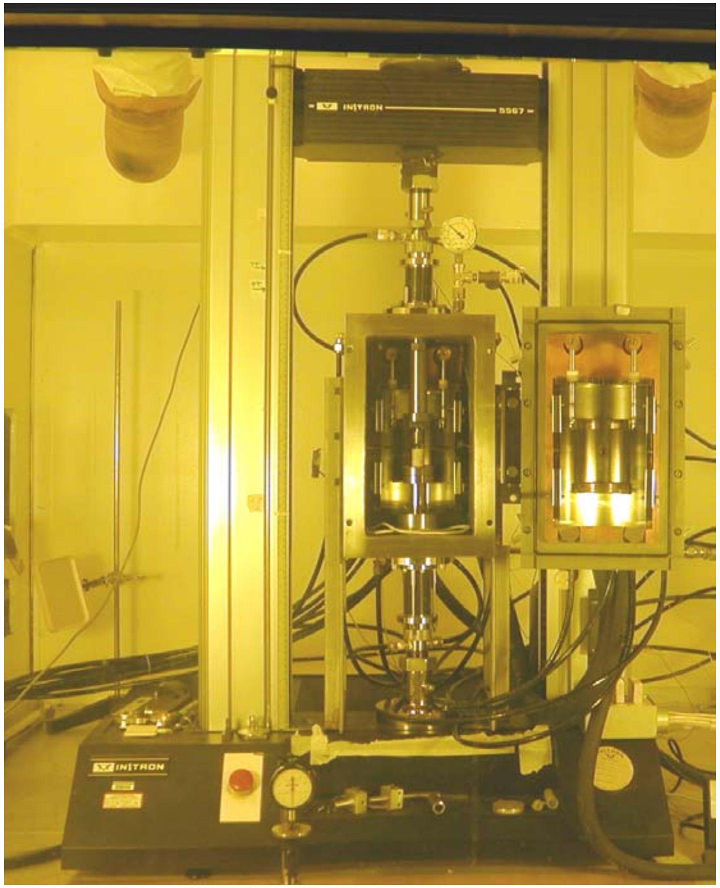
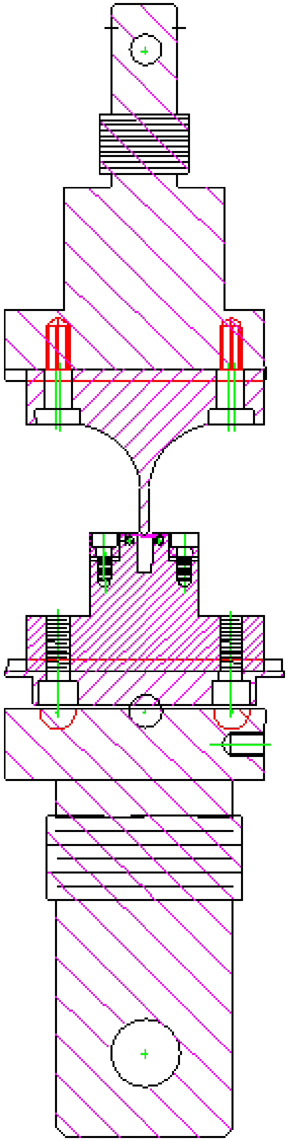
Goals/Objectives

- Determine the effect of high energy proton and neutron irradiation on the mechanical properties of structural materials for the AFCI project under prototypical conditions of irradiation temperature and flux.
  – Irr. Temperature 400-600ºC
  – Total fluence up to 200 dpa
  – Materials
    » T91, HT-9, EP823
    » 316L
    » Backup solid target-tungsten/tantalum
- Use mechanical test data to determine structural design allowables for AFCI components.
- Support Gen IV materials program
  – Testing of FFTF irradiated specimens
  – Collaborating with testing plans

3 pt. Bend Testing





- Specimen size used is 2 mm x 8 mm x 0.25 mm thick
- Specimen sliced from proton irradiated rod and ground and polished in hot cell.
- Tested at equivalent strain rate of 10^{-3}/s in outer fiber.
- Tested at 250C, 350C and 500C in ultra high purity argon.

$$\sigma = {1.5PL}/{bh^2}$$

$$\varepsilon = {6 * h * \delta}/{L^2}$$

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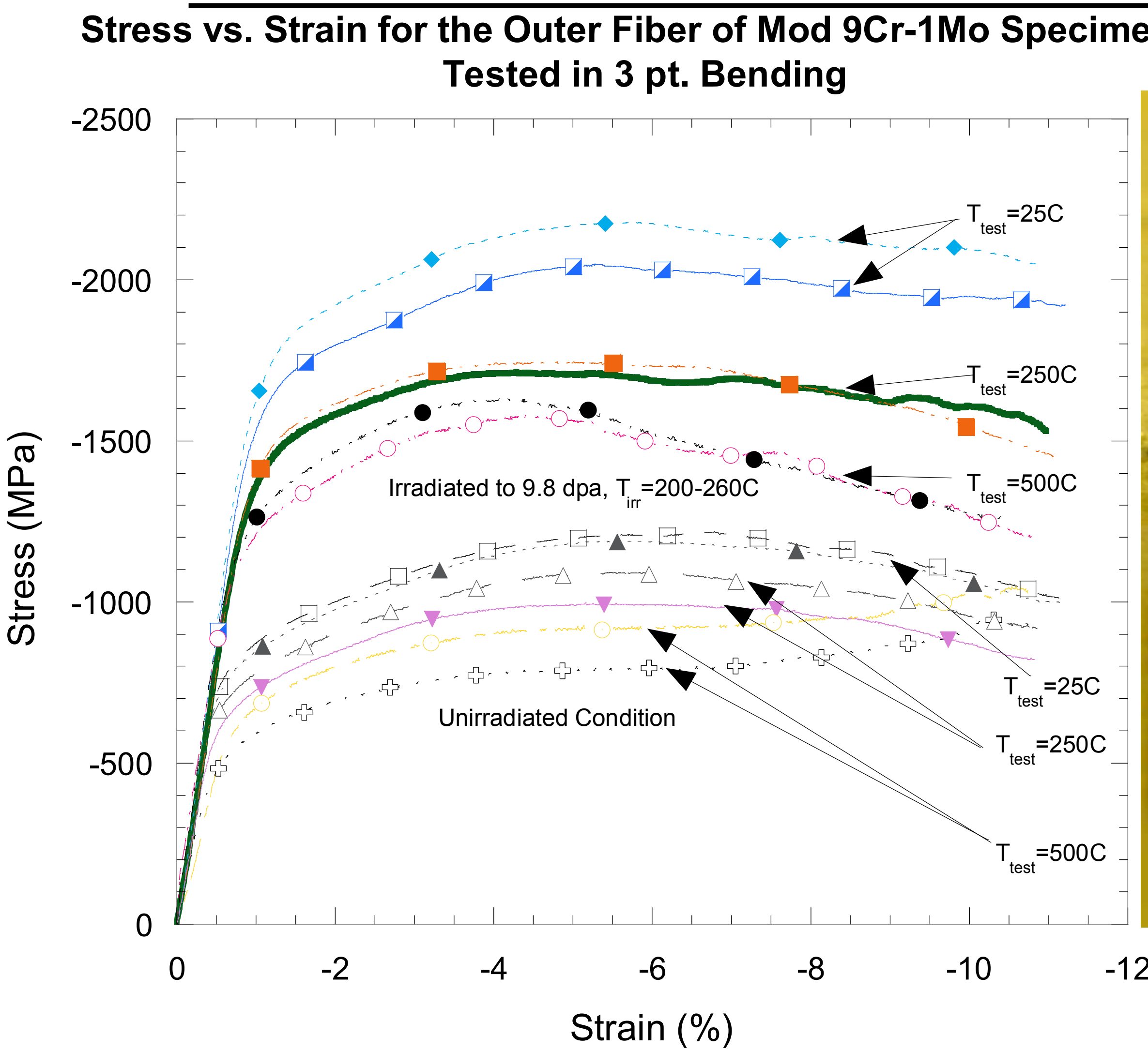
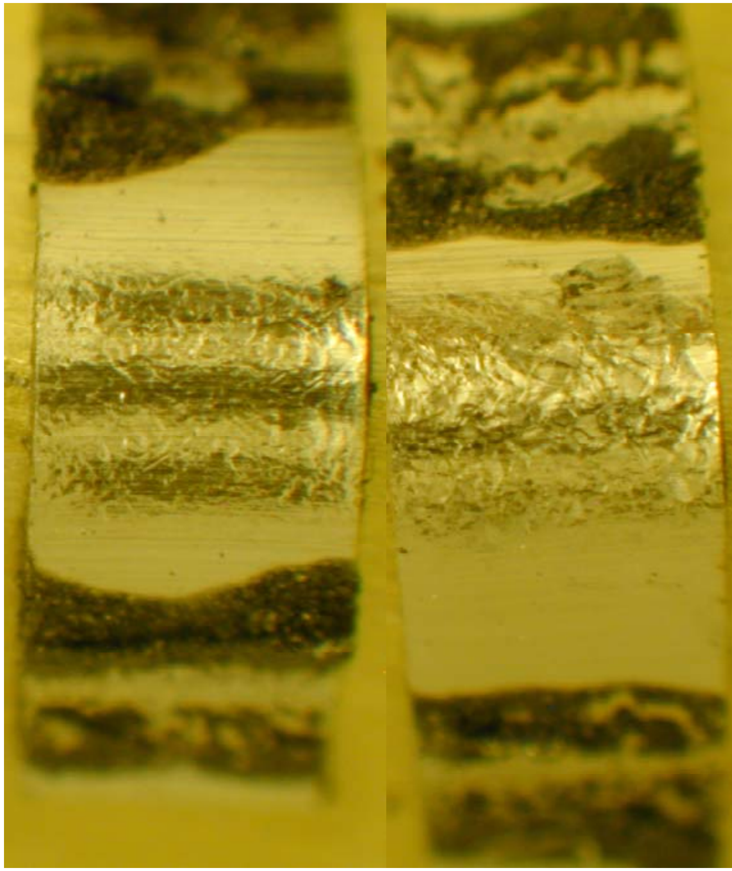
3 pt. Bend testing of Mod 9Cr-1Mo



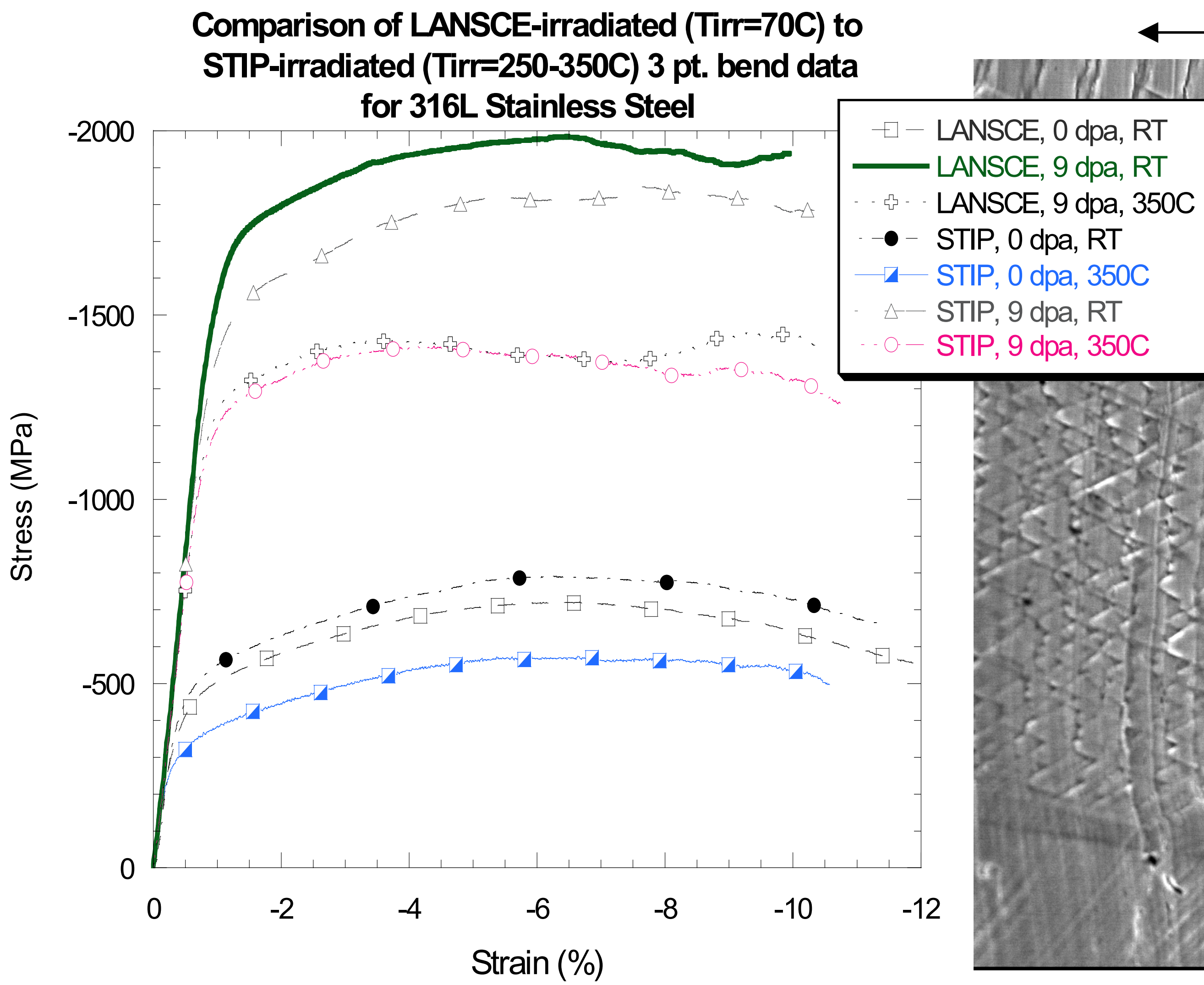


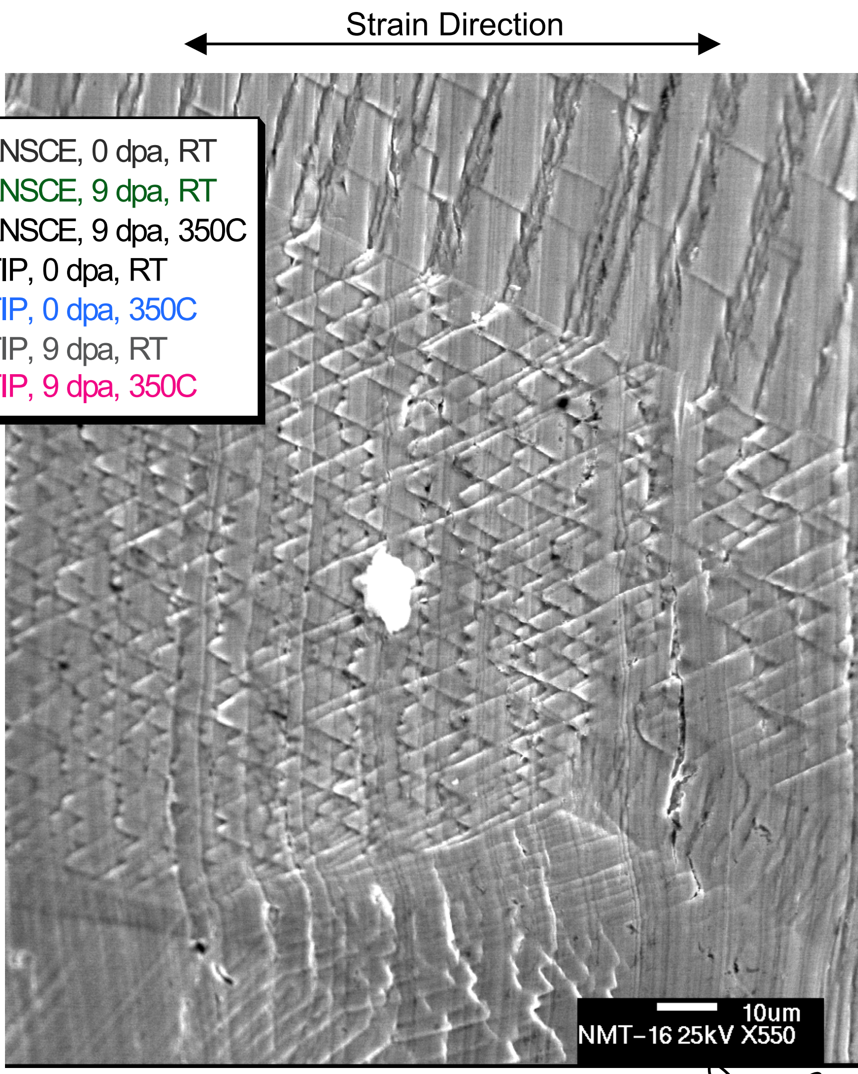
Unirradiated

Irradiated (9.8 dpa)

Tested at 500C

3 pt. Bend testing of 316L Stainless Steel

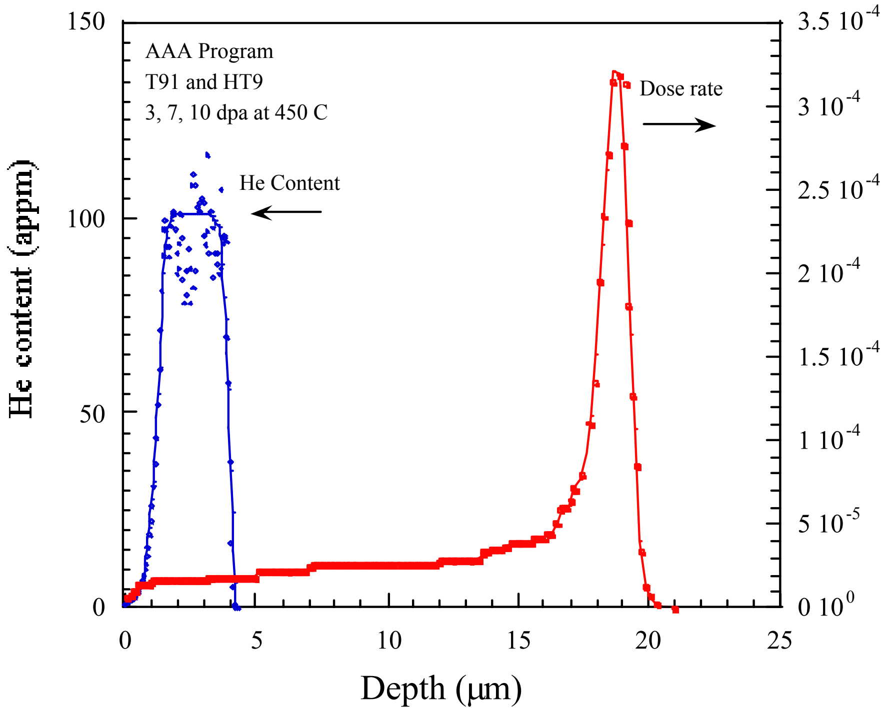


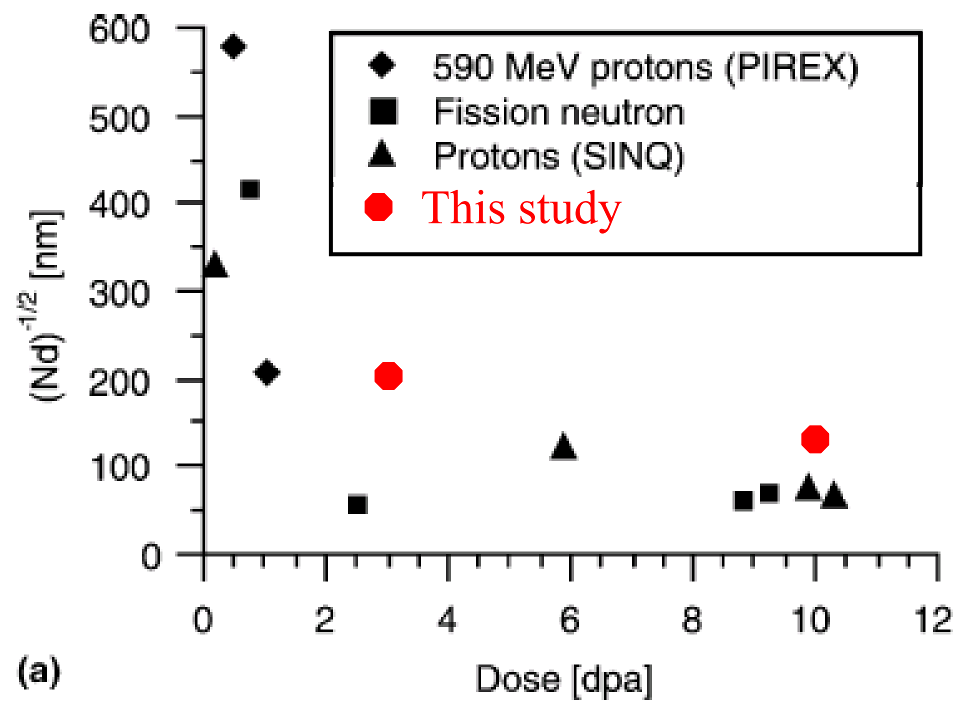


STIP, 9 dpa, 350C

Ion Irradiations on 9Cr-1Mo at University of Michigan

MichiganEngineering
1854 - 2004





F82H irradiated at ~ 310°C.

- **Microstructure (plotted as mean loop spacing) agrees well with F82H irradiated with both spallation and fission sources.**
- **Higher loop spacing is in agreement with higher irradiation temperature.**

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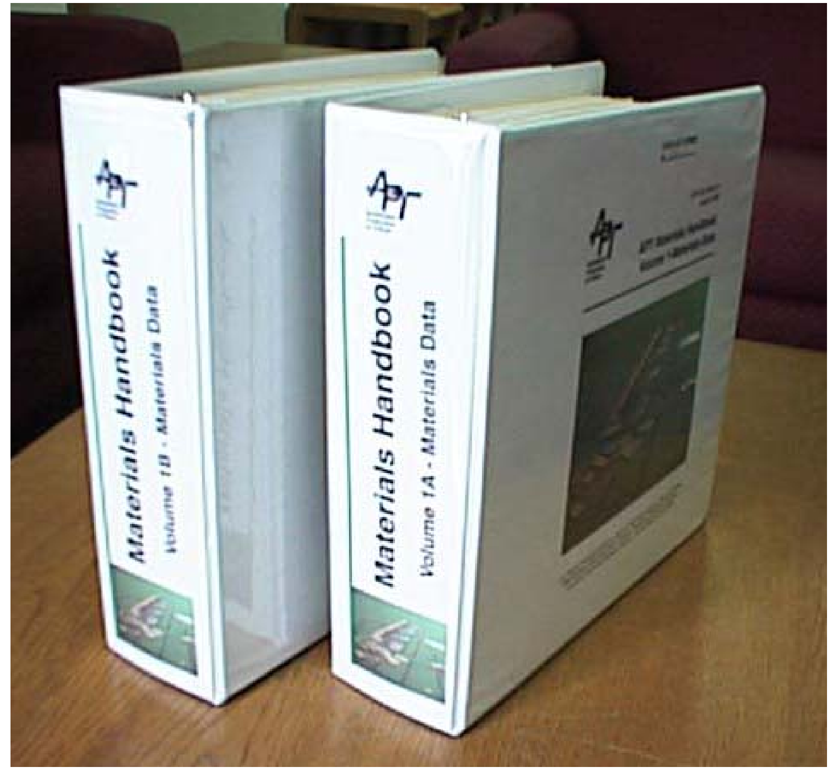
Two Major Activities Were Completed for the *Materials Handbook*

Review and final revisions to Chapter 21 on Tantalum were Completed

- Original draft of the chapter was prepared by Hans Ullmaier of the ESS Project at Forschungszentrum Juelich

Handbook Chapter 18 on HT9 ferritic/martensitic stainless steel was drafted and reviewed

- First complete draft prepared by the Handbook Coordinator



  - Based on a first partial draft prepared by Todd Allen on ANL
  - Chapter includes selected information on Russian ferritic/martensitic steels of similar composition to HT9.
  - Russian steels have higher Si content to provide increased resistance to attack in Pb-Bi eutectic.

Both chapters will be ready for inclusion in Revision 4 on the *Materials Handbook* in the Fall.

Future Testing of Irradiated Specimens

- **Specimens Irradiated in FFTF (Available in FY'04)**
  - Doses up to 120 dpa
  - Irradiation Temperature= 400 to 700C
  - Specimen types: Tensile, Pressurized Tubes, Compact Tension
  - Materials: HT-9, MA957 (ODS Strengthened Ferritic/Martensitic Steel), 10Cr-1Mo, AISI 422, F82H
- **STIP II irradiation (Irradiated in 590 MeV SINQ accelerator)-Available end of FY'03**
  - Doses up to 12 dpa
  - Irradiation temperature=250-350C
  - Specimen types: Tensile, TEM
  - Materials: HT-9, EP-823, Mod 9Cr-1Mo
- **Preparing Specimens for STIP IV Irradiation-Available end of FY'06**
  - Doses up to 12 dpa
  - Irradiation temperature = 400-500C
  - Specimens types: Tensile, TEM
  - Materials
    - » Structural: HT-9, EP-823, Mod 9Cr-1Mo, ODS strengthened F/M steels, High purity Ta, single crystal Fe (for modelling studies)
    - » Fuels Matrices: ZrN, NiAl, FeAl, RuAl, MgO, Cubic ZrO_2, Fissium

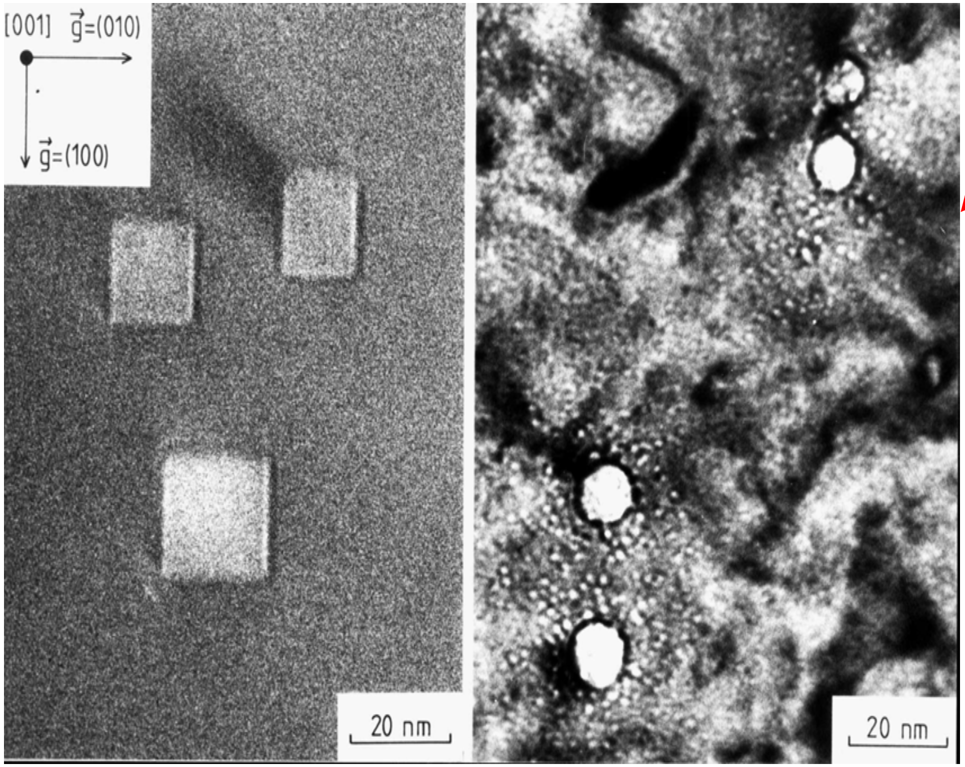
Multiscale Modeling: Generation and Evolution of Helium and Hydrogen Bubbles in Iron

Bubbles in Fe-12% Cr After 100 keV He^+ Implantation

Fe^+ irradiation to 30 dpa @ 573K

600 appm He @ 973K

600 appm He @ 973K+ 300keV



- **Halos of small bubbles around the large parent bubbles, formed by He atoms dissolved from the parent bubbles.**

Multiscale Approach to Modeling

Defect Energies
Formation energies/Geometry of atomic defects

Cascade Dynamics
Initial Damage and defect recombination
Defect diffusivities

Bubble Evolution
Brownian motion of defects to clusters
Effect of Temperature/ defect ratios

Atomistic Calculations
First Principles Approach (VASP)
Empirical MEAM potentials

Molecular Dynamics
Empirical MEAM* potentials
Integrate Newton's second law for all atoms in cascade

Kinetic Monte Carlo
Stochastic event-based simulation
Rates of KMC events parameterized by atomistic calculations/experiments

*Modified Embedded Atoms Method: Baskes et al PRB v.42 (1992)

Current Work

- **Molecular Statics**
  - Established lattice parameters for bcc Fe at 300, 373, 573, 673 K
  - Created He systems at pressures of 0.01, 1.0 and 30 kbar
  - Created He-Fe systems with d=30 angstrom voids
- **Molecular Dynamics**
  - Initiated trial low energy PKAs (5keV) in Fe
  - Initiated trial low energy PKAs (5keV) in Fe-He system (parallel machines)
  - Modified parallel code (WARP) to run displacement cascades on Q machines
  - Calculated migration energies of He in bcc Fe
- **Accelerated Molecular Dynamics**
  - Migration of He interstitial atoms in bcc Fe: in progress

Simulation of 150000 atoms. He cluster in the center of BCC iron

Linking Modeling & Experimental Efforts

Defect Energies
First Principles Calculations

Cascade Dynamics
Molecular Dynamics

Bubble Evolution
Kinetic Monte Carlo

1 10 100

Bubble Size (nm)

Irradiated samples of iron/steel

Diffraction
Defect Geometry
NMR Spectroscopy
Defect Energies

Positron Annihilation
Helium/Hydrogen content
TEM
Defect Distribution

Microstructural evolution
SEM
TEM

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*Modified Embedded Atoms Method: Baskes et al PRB v.42 (1992)

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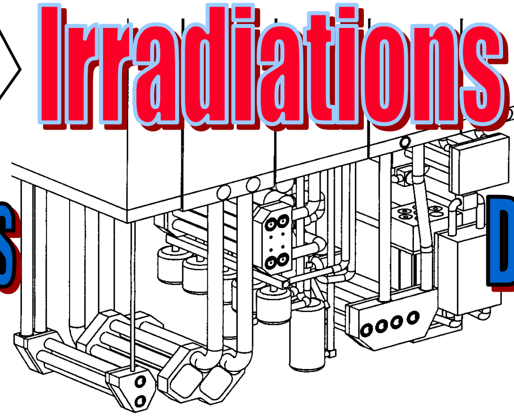
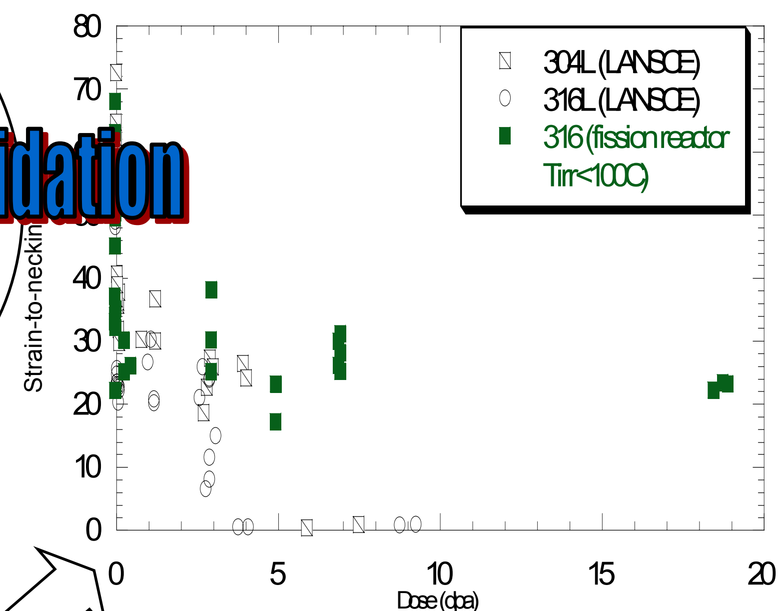
Vision for the Future

Irradiations



Data Needs

Data Validation



Predictive Models

Design New Materials

Prediction of Properties

Predict Material Lifetimes

Issue:
Irradiation Facility: No facility in US for Fast Reactor or High Energy Proton Irradiations.

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Future Plans ('04)

- Mechanical Testing and Microstructure
  - Test Mechanical Properties of FFTF irradiated specimens at 400-600C.
  - Test Specimens irradiated at PSI (STIP II irradiation) at 400-600C
- Data
  - Incorporate new data into next revision of Materials Handbook
    - » FFTF Irradiated Specimens
    - » STIP Irradiated Specimens
  - International Collaborations
    - » TRADE target
    - » Megapie PIE
    - » CEA
- Atomistic Modeling of He in Body-centered Cubic (BCC)-Fe
  - Examine cascade interactions with He/H bubbles.
  - Examine grain boundary interactions with defects.
  - Evolution of gas bubbles employing data from molecular static/dynamics calculations
  - Look at the effect of defect ratios and temperature on gas bubble evolution.
  - Benchmark calculations with experimental results